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AD822301

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DETONATION CALCULATIONS

by

Julius Roth

AUGUST 1967

SRI Project PAU-4900

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Special Technical Report No. 13

by

Julius Roth

AUGUST 1967

DEPARTMENT OF THE ARMY
EDGEWOOD ARSENAL
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Edgewood Arsenal, Maryland 21010

STANFORD RESEARCH INSTITUTE
Menlo Park, California

FOREWORD

The work described in this report was authorized under Task 1B522301A08101, "Dissemination Investigations of Liquid and Solid Agents (U)." The work was started in April 1964 and completed in August 1967.

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DIGEST

Flashing of agents during the dissemination process reduces the effectiveness of chemical munitions. Afterburning of detonation products of the explosive charge appears to trigger flashing, i.e., the ignition of agent-air mixtures. The chemical composition of the explosive charge detonation products controls the ignitibility of product/air mixtures. If product/air mixtures cannot burn, one of the main causes of flashing will have been eliminated.

At present detonation product composition cannot be obtained experimentally. They can only be estimated by theoretical calculations, some of which are based on inadequate or even invalid assumptions. Consequently, the objective of this effort was to choose the most plausible of the currently available theoretical calculations and to use it in estimating product compositions of likely dissemination charges. Additionally, such calculations provide estimates of other detonation parameters, such as temperature and pressure, which may also be important in some facets of the dissemination process.

The computational scheme adopted was RUBY. It was used to estimate detonation parameters for Comp B, Comp B/oxamide, amatols, HMX, HMX/AP, and HMX/AN. Based on these calculations explosive charges for diagnostic tests of agent degradation are suggested.

3

CONTENTS

ILLUSTRATIONS

TABLES

8

I INTRODUCTION

A. Objective and Outline of Approach

Chemical agents may degrade during their dissemination by high explosive munitions. One of the more spectacular forms of agent degradation, though not necessarily the only one, is called "flashing." As the term implies, flashing refers to the formation of a fireball of burning agent and high explosive detonation products. Clearly, flashing or other degradation reduces the effectiveness of a chemical munition. Consequently, the objective of SRI's overall program is the elimination of agent degradation. The particular phase of the program reported here deals with the early stages of the dissemination process, namely, the interaction of high explosive detonation products with the agent. Calculation of detonation parameters such as product composition and temperature could lead to (1) a rational understanding of the role of the high explosive in the flashing process, (2) suggestions of explosive compositions for diagnostic tests of flashing or other degradation mechanisms, and (3) suggestions for practical explosive compositions that will minimize flashing.

We will review the methods of calculating detonation parameters and we will demonstrate why the so-called RUBY code[1] method, although by no means free of shortcomings, appears to be the best calculational method currently available. We will then present the results of RUBY calculations of the explosives now used in chemical munitions and calculations for explosives which we believe will minimize flashing. As this presupposes an understanding of the flashing process, some justification of the hypotheses adopted for the flashing process will be appropriate at that stage of the report. Explosives for diagnostic tests of the various flashing mechanisms will be proposed. Finally, we will suggest a practical explosive composition that should minimize flashing and we will present some recommendations for improving detonation calculations.

B. General Review of Detonation Calculations

Anyone involved in the design or procurement of munitions will, at some time, be faced with a set of calculated detonation parameters. Unfortunately, there is no general agreement on how these calculations should be made, nor is there general agreement in the results of the calculations. Thus, a munition designer must decide for himself which calculations he should believe. Because of its direct bearing on our immediate objective of preventing agent flashing, we will present here a brief state-of-the-art review of detonation calculations.

All detonation calculations assume equilibrium conditions; i.e., all the chemical and hydrodynamic effects are assumed to have reached a steady state. Usually calculations are carried out for one-dimensional detonations so that the complicated effects of divergent flow can be neglected. In common practice truly one-dimensional detonation is approached only in the central regions of a sizable explosive charge, at a considerable distance from the point of initiation. For a steady one-dimensional wave it is then possible, in principle, to calculate all the detonation parameters (detonation velocity, particle velocity, pressure, temperature, specific volume, and product composition) from conservation of mass, conservation of momentum, conservation of energy, an equation of state for the detonation products, the thermochemistry of products and reactants, and the Chapman-Jouguet condition. The Chapman-Jouguet condition requires that, at equilibrium, $D = C + u$, where D is the detonation velocity, C is the local sound velocity, and u is the particle velocity. Assuming detonation products are perfect gases and neglecting the difference between the initial pressure and the final pressure, these conditions lead to

$$\rho_1/\rho_0 = \frac{\gamma_1 + 1}{\gamma_1} \tag{1}$$

$$P_1 = 2\rho_0 Q_1 (\gamma_1 - 1) \tag{2}$$

$$T_1 = \frac{Q_1 \gamma_1}{(\gamma_1 + 1)c_1} \tag{3}$$

10

where ρ is density, γ is the ratio of the specific heat at constant pressure and constant volume, P is pressure, Q is heat of reaction per gram of explosive, T is temperature, and c is specific heat at constant volume. The subscript 1 refers to the equilibrium detonation state, and the subscript 0 refers to the original, unreacted explosive.

Other equations for detonation velocity or particle velocity are readily obtainable, but for the moment we will devote our attention to the three equations above, since they serve to illustrate how a detonation calculation proceeds, how the calculation is improved by correcting for gas imperfections (detonation products of condensed explosives are anything but perfect gases), and how the equations can be used for making estimates of variations in the detonation parameters produced by changes in the chemistry of the process (e.g., changes in the heat of reaction or the number of moles of gas in the products). As an example, consider the detonation of acetylene in oxygen, where all products are assumed to behave as perfect gases but there is insufficient oxygen to produce solely H_2O and CO_2. We might expect the net reaction to be something as follows:

$$C_2H_2 + 2O_2 = CO_2 + CO + H_2O$$

If this equation gives the actual product composition, then the problem of obtaining detonation parameters is nearly solved. The known products and reactants determine Q_1, according to

$$Q_1 = \sum_i (n_i \Delta H_f^o)\text{products} - \sum_j (n_j \Delta H_f^o)\text{reactants},$$

where n is the number of moles per gram of the i-th and j-th species and ΔH_f^o is the standard heat of formation. The known products determine c_1 and γ_1. Thus, all the necessary information is available to solve Eqs. (1) through (3). Even for ideal gas behavior, however, the products are not necessarily those given by a balanced chemical equation. For our example, we would certainly have to consider that the products rearrange according to the water gas equilibrium,

$$CO_2 + H_2 = H_2O + CO \tag{a}$$

11

which is temperature-controlled. The products may also dissociate according to

$$CO_2 = CO + 1/2 \ O_2 \qquad\qquad (b)$$

which is both temperature- and pressure-dependent. Thus reaction (a) leads to

$$K(T) = \frac{p(H_2O)p(CO)}{p(CO_2)p(H_2)}$$

and reaction (b) leads to

$$K(T,p) = \frac{p(CO)p(O_2)^{1/2}}{p(CO_2)P_1^{1/2}}$$

where K is a thermodynamic equilibrium constant, p is partial pressure, and P_1 is the total pressure at equilibrium. In making the calculation we assume an equilibrium temperature and pressure, and with the appropriate equilibrium constants for these assumed conditions we calculate the product composition. Based on this composition we obtain Q_1, c_1, and γ_1 and solve Eqs. (1) through (3). Using the calculated T_1 and P_1, we repeat the equilibrium calculations and use the new composition to recalculate T_1, P_1, etc. This is repeated until the assumed and calculated temperatures and pressures are brought into agreement. It should be realized immediately that, aside from any other effects on Eqs. (1) through (3), gas imperfections will affect the equilibrium calculations since the partial pressures in the equilibrium expressions will have to be replaced by fugacities[2] (probably unknown for the regions of interest of products from condensed explosives). In addition, the total pressure terms, such as the one in the dissociation of CO_2, will be much larger for the highly imperfect gases than for ideal gases.

The effect of gas imperfections can be even more drastic on Eqs. (1) through (3) than it is on the equilibrium calculations. One of the simplest imperfection corrections that can be made is to assume that the

product gases are rigid spheres occupying a definite volume, the so-called co-volume α, which is independent of temperature and pressure. This leads to the Abel equation of state (a simplification of Van der Waals' equation) and transforms Eqs. (1) through (3) into

$$\frac{v_1}{v_0} \approx \frac{k_1 + \alpha/v_0}{k_1 + 1} \tag{4}$$

$$P_1 = \frac{2Q_1(k_1 - 1)}{v_0 - \alpha} \tag{5}$$

$$T_1 = \frac{2Q_1 k_1}{(k_1 + 1)c_1} \tag{6}$$

where $v = 1/\rho$ and $k_1 = 1 + (n_1 R/c_1) = \gamma_1$ if $\alpha =$ constant.

Comparison of this set of equations with Eqs. (1) through (3) shows that if product composition is essentially unaffected by the gas imperfections considered (i.e., Q_1 and c_1 are essentially the same for Abel and ideal products), then the only parameter that is appreciably altered is P_1 in the sense that $(P_1)_{Abel} > (P_1)_{ideal}$. Theoretical considerations, as well as lack of agreement between calculated and observed detonation parameters, make untenable the assumption of an α independent of p and v. Several attempts have been made to improve the Abel equation by removing the restriction that α be constant. Cook[3] has made extensive calculations using a PvT equation of state of the type

$$Pv = nRT + \alpha(v)P \tag{7}$$

where $\alpha(v)$ is obtained from experimental measurements of detonation velocity. A variation of the form of Eq. (7) has been obtained independently by Paterson[4] using an essentially "first principles" (cell theory) approach rather than the empirical approach of Cook. Paterson's equation of state is

$$Pv = nRT[1 + (b/v) + 0.625(b/v)^2 + 0.287(b/v)^3 + 0.193(b/v)^4] \tag{8}$$

13

where $b = \sum_i n_i b_i$, and b_i, the second virial coefficient of the i-th gas species, is assumed constant. Extensive calculations using Paterson's method are given by Taylor.[5] Since the calculations require measured detonation velocities and the variation of detonation velocity with loading density of the explosive, another empirical approach, that of Jones,[6] is based on an equation of state identical with Eq. (7) except that $\alpha = \alpha(P)$ and not $\alpha = \alpha(v)$.

The cell theory equation of state of Lennard-Jones and Devonshire, usually called LJD, was used for detonation state calculations by Fickett.[7] Fickett's treatment, though subject to some criticism on theoretical grounds, leads to certain results, confirmed by experiment, that are not obtainable by other calculational methods now used.

The so-called BKW equation of state, upon which RUBY code is based, was put into its present form largely by Cowan and Fickett[8] and by Mader.[9] It is semiempirical in nature and takes the form of

$$\frac{Pv}{RT} = 1 + Xe^{\beta X} \qquad (9)$$

where

$$X = \frac{\displaystyle \oint \Sigma \, n_i \alpha_i}{v(T + \theta)^a}$$

The quantities a, β, and θ are adjustable parameters that are intended to be universal constants. ⱪ is a scaling factor and α_i is the co-volume of the i-th gas species. β and ⱪ are adjusted to make the calculated detonation velocity and its variation with packing density fit the experimental observation on a "standard" explosive. Then "a" is chosen to reproduce the observed pressure of the "standard." Since pressure would go to infinity when $T \to 0$, a factor θ is introduced into Eq. (9). The parameters, a, β, ⱪ, and α_i have been frequently reevaluated and readjusted. Thus some confusion exists among calculations done at different times and at different facilities. Currently, Mader[9] uses two "standards"--RDX and TNT--with some different "constants" for each standard.

II CALCULATIONS

A. Merits and Shortcomings of BKW Equation of State

Calculations based on Abel's, Cook's, or Paterson's PvT equations
of state are in principle applicable only to thermodynamically ideal mix-
tures since these methods neglect the energy of gas imperfections. It is
to be expected that detonation products of condensed explosives ("gases"
such as CO_2, N_2, and H_2O at densities greater than the packing density of
the original explosive) are far from thermodynamically ideal. As these
calculations do not consider any repulsion energy of the detonation prod-
ucts, the detonation temperatures they generate will be too high, since
the entire chemical and hydrodynamic energy increase appears as an in-
crease in temperature of the detonation products. Because the adjustable
parameters of all previously mentioned computational procedures were chosen
to fit experimentally observed detonation velocities (sometimes also det-
onation pressures), and in view of the fact that calculated velocities,
and to a lesser extent pressures, are rather insensitive to the form of
the PvT equation of state, it is not at all surprising that these proce-
dures are successful in predicting detonation velocities and detonation
pressures. A much more severe test of the validity of a computation scheme
is to be found in comparing calculated detonation temperatures and product
compositions with experiment. Unfortunately, for condensed explosives
there are few (and some may claim no) unambiguous experimental detona-
tion temperatures and certainly no product compositions measured at the
detonation equilibrium state.

Thus the choice among existing PvT equations of state for any com-
putational scheme should be made primarily on the basis of fundamental
physics. Consequently, schemes that allow for intermolecular energy
should be considered more plausible than procedures that neglect it.
Fickett's treatment of the LJD equation of state[7] may suffer somewhat
from an inadequate approximation for treating gas mixtures (detonation
products are usually mixtures and not single species). In addition,

the dependence of repulsion energy on intermolecular separation may not have been expressed in a manner that agrees best with theory; nevertheless, his treatment qualitatively predicts the shape of the adiabatic exponent (along an isentrope through the equilibrium detonation state) versus expanded volume curve actually observed for several explosives.[10] Unfortunately, Fickett's method is not readily adaptable to fairly routine calculations.

The BKW equation of state allows only forces of intermolecular repulsion and completely neglects any forces of intermolecular attraction. Thus, the BKW equation certainly underestimates detonation temperature and is inadequate for isentrope expansion calculations; however, in its RUBY code form[1] it does lend itself to routine calculations. The detonation temperatures and the product composition for oxygen-poor explosives obtained from RUBY must be taken with a considerable amount of skepticism. It is possible, however, that RUBY, though it errs in absolute values of temperature and composition, correctly predicts relative values. In any event RUBY calculations, with all their shortcomings, are still more plausible than computations based on the several variants of the Abel equation.

For many military explosives at near maximum loading density, Mader[9] calculates $T_1 \approx 2500^0 K$ while Cook[3] calculates $T_1 \approx 5000^0 K$. The P_1's calculated by both methods are roughly the same. Let us examine how the differences in T_1 affect equilibrium product composition. Because of the high detonation pressures, dissociation reactions of the type $CO_2 = CO + 1/2 \, O_2$ will be repressed, although Cook (because of his higher T_1) will favor dissociation. In the so-called soot reactions,

$$2CO = CO_2 + C_{(s)} \qquad\qquad (c)$$

$$CO + H_2 = H_2O + C_{(s)} \, , \qquad\qquad (d)$$

high pressure favors the formation of solid carbon. The following tabulation shows that for a given pressure the soot reactions will be greatly enhanced by low T_1's:

Reaction	Thermodynamic Equilibrium Constants	
	At 2500°K	At 5000°K
(c)	3.4×10^{-3}	1.3×10^{-7}
(d)	2.7×10^{-2}	1.6×10^{-3}

Large amounts of soot are commonly observed in the products of detonation of military explosives. There is some evidence that the soot is largely in the amorphous rather than in the graphitic carbon form. It is interesting to estimate to what extent calculated detonation product compositions depend on the form of the solid carbon. Even more important would be estimates of how incomplete precipitation of solid carbon affects product composition. Such incomplete precipitation may be one of the most common causes of the failure of an actual detonation to reach thermodynamic equilibrium. Figure 1 presents RUBY calculations for Comp B under different assumptions for the fate of product carbon. It is obvious from Fig. 1 that the form of the solid carbon--amorphous or graphitic--has little effect on product composition. For the extreme case of no
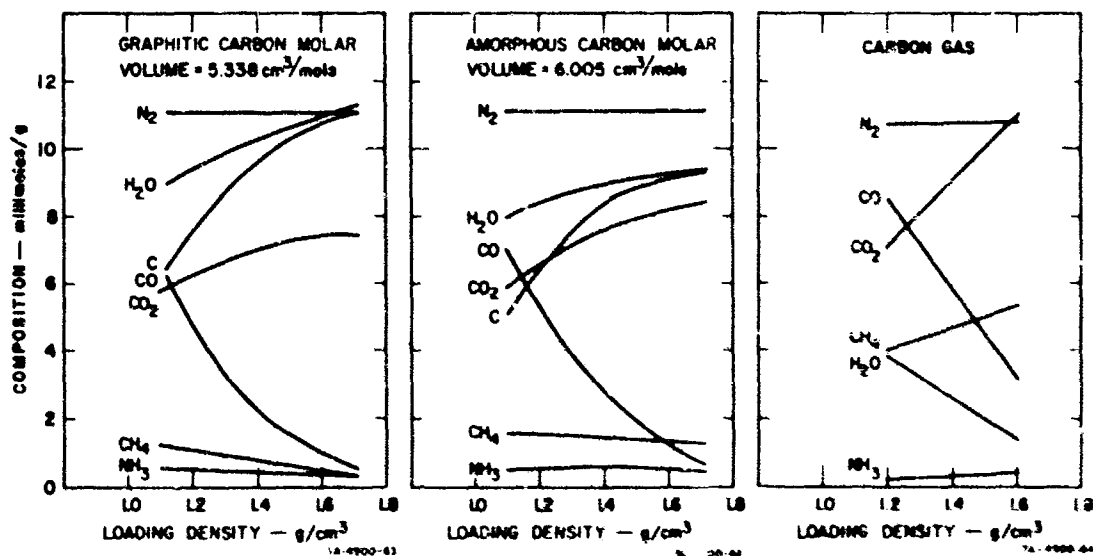

FIG. 1 PRODUCT COMPOSITIONS FOR COMP B-3 CALCULATED
UNDER THREE ASSUMPTIONS CONCERNING CARBON

carbon precipitation the products become richer in CH_4 and CO_2 primarily
at the expense of H_2O. For conditions favoring soot reactions (oxygen-
deficient explosives at high packing density), one can make fairly ac-
curate estimates of the detonation product composition merely by allow-
ing all the hydrogen atoms of the original explosive to form H_2O, with
any remaining oxygen combining with the initially present carbon to form
CO_2. Any carbon left over will appear as solid carbon in the products
and any nitrogen atoms originally present will form N_2. As an example,
consider RDX. At high loading density the reaction

$$C_3H_6O_6N_6 \rightarrow 1.5\ CO_2 + 3\ H_2O + 3\ N_2 + 1.5\ C_{(s)}$$

is much favored over the reaction

$$C_3H_6O_6N_6 \rightarrow 3\ CO + 3\ H_2O + 3\ N_2$$

B. Comparison of RUBY with Experiment

It has already been mentioned that T_1 is much more sensitive to the
choice of a PvT equation of state than P_1. Unfortunately, completely
unambiguous experimental T_1's are not available. Experimental tempera-
tures for granular explosives must be considered much less reliable than
experimental temperatures for clear liquid explosives because of "detona-
tion light"[11] and air shock due to air inclusions. In Table I published
experimental values of T_1 and P_1 are compared with Mader's[9] BKW calcula-
tions. (Mader has done more "curve-fitting" and has published calcula-
tions for a wider variety of explosive compositions than have RUBY users.)
There is some disagreement in experimental temperatures and somewhat less
disagreement in experimental pressures. As expected, measured and
calculated pressures agree well. For liquid explosives, the temperatures,
calculated and experimental, agree within $150^\circ K$ in three instances; the
lowest experimental values are at least $250^\circ K$ higher than the calculated
in four cases, and in two cases they are appreciably lower than calculated
values. Thus, when allowance is made for the uncertainty in measured det-
onation temperature, RUBY calculations and experiments are in reasonable

18

Table I

COMPARISON OF RUBY CALCULATIONS WITH EXPERIMENTS

Explosive	ρ_o (g/cc)	Oxygen Balanced[a]	P_1 Observed (kbar)	P_1 Calculated (kbar)	T_1 Observed (°K)	T_1 Calculated (°K)
NG	1.59	+ 3.5	253[b]	246	3470 / 4000[c] / 4000[d]	3216
NM	1.13	−39.4	~1±7 / 129[b]	130	3380 / 3380[e] / 3700[c] / 3800[d]	3120
TNM	1.64	+49.0	159	162	2800	1341
TNM	1.64	+49.0	159	162	3100[c]	1341
NM/TNM 1/0.071	1.20	−22.8	138	153	3480	3354
NM/TNM 1/0.25	1.31	0	156	181	3750	3998
NM/TNM 1/0.50	1.40	+16.8	168	191	3580	3565
Acrylonitrile/ TNM 1/1.25	1.38	0	156	192	4000	4760
EtNO₃	1.11	−61.5	−	133[f]	3130[e]	2645[f]
PETN(s)	1.77	−10.0	342[c]	319	4200[c]	2833
PETN(s)	1.67	−10.0	> 300±6	280	3400 ± 400	3018
Dina(s)	1.70	−27.0	−	303[f]	3700[c]	2577[f]
Tetryl(s)	1.70	−47.4	283[c]	251	2950[c]	2917
RDX(s)	1.80	−22.0	347	347	3700[c]	2587
	1.80		354[b]	347		
	1.80		392[c]	347		
	1.40		213[b]	200		3272
	1.20		152[b]	149		3478

Table I (Concluded)

Explosives	ρ_o (g/cc)	Oxygen Balance[a]	P_1		T_1	
			Observed (kbar)	Calculated (kbar)	Observed (°K)	Calculated (°K)
TNT(s)	1.64	-77	209	206		
	1.60		202[b]	194		
	1.45		178±13	157		
			162[b]			
	1.00		64[b]	76		
TNT(l)	1.45	-77	182[f]	157	3030	3126

Note: all results without footnotes as well as all calculations (unless indicated) from Mader.[9]

(a) Oxygen balance $= -\dfrac{1600}{\text{formula wt}} \left[2C \text{ atoms} + \dfrac{H}{2} \text{ atom} - O \text{ atom.} \right]$

(b) A. N. Dremin and P. F. Pokhil, Doklady 128(5), 989 (1959).
(c) I. M. Voskoboynikov and A. Ya. Apin, Doklady 130(4), 804 (1960).
(d) F. C. Gibson et al., JAP 29, 628 (1958).
(e) J. T. A. Burton and J. A. Hicks, Nature 202, 758 (1964).
(f) W. C. Davis, B. G. Craig, and J. B. Ramsey, "Failure of the Chapman-Jouguet Theory for Liquid and Solid Explosives," Preprints, Fourth Symposium on Detonation, Vol. I, 1965, p. A-50.
(g) D. Price and H. Hurwitz, Ref. 12.

agreement, although one may detect a tendency for RUBY temperatures to be lower than observed temperatures.

C. Comparison of Calculations at Different Facilities

As already mentioned, the parameters of the BKW equation (Eq. 9) have undergone some change through the years. Typical variations are shown in Table II. These variations result in the differences shown in Table VII in computed detonation properties between Los Alamos Scientific Laboratory-- Naval Ordnance Laboratory (LASL-NOL) and Stanford Research Institute-- Lawrence Radiation Laboratory (SRI-LRL). Generally, the LRL-SRI T_1 are lower and v_1 are higher than the corresponding LASL-NOL values. For

Table II

BKW PARAMETERS

Parameter	Mader[9]		SRI and LRL
	RDX Fit	TNT Fit	
a	1/2	1/2	1/2
β	0.160	0.0959	0.100
θ ($^\circ$K)	400	400	400
↓	10.91	12.69	11.85
α_1 (cc/kg)			
H_2O	250	250	360
CO_2	600	600	670
CO	390	390	:)
N_2	380	380	380
H_2	180	180	180
CH_4	528	528	528
O_2	350	350	350

comparison this table also includes Cook's (based on Eq. 7), Paterson's (based on Eq. 8), and Fickett's results (based on the LJD equation of state). Compared to the Mader (LASL) or NOL[1] calculations Cook and Paterson obtain somewhat lower pressures and much higher temperatures. Fickett's results for P_1 are also lower than Mader's and his T_1's are between those of Mader and Cook. Equilibrium product compositions obtained by Mader are compared to our calculations in Table IV. Generally Mader's results show a little more solid carbon than ours (at the expense of CO_2 and CO and more H_2O (at the expense of minor products such as CH_4 and NH_3).

Table III

TYPICAL CALCULATED DETONATION PARAMETERS

Calculated by	Explosive	ρ_o	D (mm/μsec)	P_1 (kbar)	T_1 (°K)	v_1 (cm³/g)
LASL (BKW Code)	TNT	1.64	7.197	206	2940	0.451
NOL RUBY			7.287	222	2740	0.452
LRL			7.115	220	2180	0.627
SRI			7.245	216	2110	0.640
Cook			–	175	4100	–
LJD-Fickett			6.880	183	3660	–
Paterson		1.5	6.450	110	3870	0.55
LASL (BKW Code)	TNT	1.00	5.161	76.2	3200	0.714
NOL RUBY			–	––	–	–
LRL				––	–	–
SRI			–	–––	–	–
Cook			–	62	3580	–
LJD-Fickett			–	–	–	–
Paterson			4.400	44.2	3870	0.769
LASL (BKW Code)	NG	1.60	7.700	346	3220	0.464
NOL RUBY			7.590	249	31??	0.458
LRL			–	–	–	–
SRI			–	–	..	–
Cook			–	250	6170	–
LJD-Fickett			7.286	208	4680	–
Paterson			8.060	199	5640	0.505
LASL (BKW Code)	Comp B	1.72	8.084	284	2760	0.435
NOL RUBY			8.100	290	2730	0.427
LRL			8.074	281	2310	0.368
SRI			8.150	283	2290	0.572
Cook			–	230	4160	–
LJD-Fickett			7.987	259	3963	–
Paterson			–	–	–	–

Table III (Concluded)

Calculated by	Explosive	ρ_0	D (mm/μsec)	P_1 (kbar)	T_1 (°K)	v_1 (cm³/g)
LASL (BKW Code)	RDX	1.80	8.754	347	2590	0.416
NOL RUBY			8.567	341	2370	0.412
LRL			–	–	–	–
SRI			8.791	353	2470	0.523
Cook			8.84	278	5040	0.450
LJD-Fickett			8.796	324	4040	–
Paterson			–	–	–	–
LASL (BKW Code)	PETN	1.77	8.421	319	2830	0.421
NOL RUBY			8.337	324	2810	0.414
LRL			–	–	–	–
SRI			8.575	339	2690	0.413
Cook			8.47	260	5630	0.453
LJD-Fickett			–	–	–	–
Paterson			–	–	–	–
LASL (BKW Code)	PETN	1.20	6.599	144	3590	0.603
NOL RUBY			–	–	–	–
LRL			–	–	–	–
SRI			6.747	156	3440	0.552
Cook			6.40	120	5310	0.630
LJD-Fickett			–	–	–	–
Paterson			6.60	118	5200	0.620
LASL (BKW Code)	HMX	1.90	9.159	395	2360	0.396
NOL RUBY			8.895	382	2510	0.392
LRL			9.084	388	2140	0.374
SRI			9.110	390	2270	0.373
Cook			–	–	–	–
LJD-Fickett			–	–	–	–
Paterson			–	–	–	–

23

Table IV

CALCULATED PRODUCT COMPOSITIONS

(mole %)

Product	HMX (ρ_0 = 1.6 g/cc)		TNT (ρ_0 =1.6 g/cc)		TNT (ρ_0 =1.2 g/cc)		RDX (ρ_0 ≈1.8 g/cc)	
	LASL	SRI	LASL	SRI	LASL	SRI	LASL	SRI
CO_2	1ა.9	17.8	14.9	19.4	11.4	17.1	16.5	18.0
CO	1.5	2.6	2.1	1.3	9.5	7.7	0.2	1.0
CH_4	-	1.4	-	2.7	-	3.2	-	0.8
$C_{(s)}$	15.9	14.2	46.7	44.1	42.8	40.2	16.5	14.4
H_2O	33.3	30.6	22.7	17.7	22.4	16.6	33.3	31.3
H_2	-	-	-	-	0.2	0.3	-	-
NH_3	-	1.2	-	0.7	-	0.7	-	0.9
N_2	33.3	32.2	13.6	14.1	13.6	14.3	33.3	33.7

D. Calculations for Comp B and Comp B-3/Oxamide

The dissemination charge presently used is Comp B-3. Consequently, it is important to estimate its detonation parameters and product composition. Using the input parameters of Table V, the results of the calculation are shown as functions of loading density in Figs. 2 and 3.

It has been suggested[13] that an explosive charge consisting of 90/10 weight percent (all subsequent compositions will be given in weight percent) of Comp B/oxamide could minimize flashing because T_1 is expected to be less for this mixture than for Comp B. That this appears to be so is also shown in Figs. 2 and 3. Note, however, that the product composition of Comp B is the same as the product composition of 90/10 Comp B/oxamide. Thus the combustibility of the products for the two explosives is the same, but the lower temperature can be expected to reduce the probability of product ignition in the case of the oxamide mixture. The 90/10 Comp B/oxamide composition does not eliminate flashing.[14]

Table V

CALCULATION INPUT PARAMETERS FOR EXPLOSIVE MIXTURES

Common Name	Composition (wt %)	Formula	Formula Weight	Oxygen Balance(a)	Maximum Density	Standard Heat of Formation (kcal/mole)	(kcal/g)
Comp B	64/36 RDX/TNT	$C_{4.42} H_{5.65} O_{6.00} N_{4.94}$	223.9	-40.3	1.75	+ 3.17	+0.014
Comp B/oxamide	90/10 Comp B/$C_2H_4O_2N_2$	$C_{3.89} H_{5.28} O_{5.12} N_{4.28}$	194.0	-43.7	1.75	-24.40	-1.258
Amatol	50/50 AN/TNT	$C_{1.82} H_{4.26} O_{3.78} N_{2.26}$	118.4	-28.3	1.69	-69.17	-0.585
Amatol	80/20 AN/TNT	$C_{0.57} H_{4.08} O_{3.24} N_{2.08}$	91.97	+ 1.0	1.71	-81.64	-0.888
"Ametex"	52/48 HMX/AN	$C_{0.798} H_{4.798} O_{3.998} N_{3.197}$	123.2	+ 0.4	1.81	-66.29	-0.538
"Chlorex"	61.2/38.8 HMX/AP	$C_{1.54} H_{5.53} O_{5.53} N_{3.70} Cl_{0.62}$	185.3	0	1.92	-35.84	-0.192

(a) Oxygen balance $= - \dfrac{1600}{\text{formula wt}}$ [2C atoms $+ \dfrac{H}{2}$ atom $-$ O atom.]
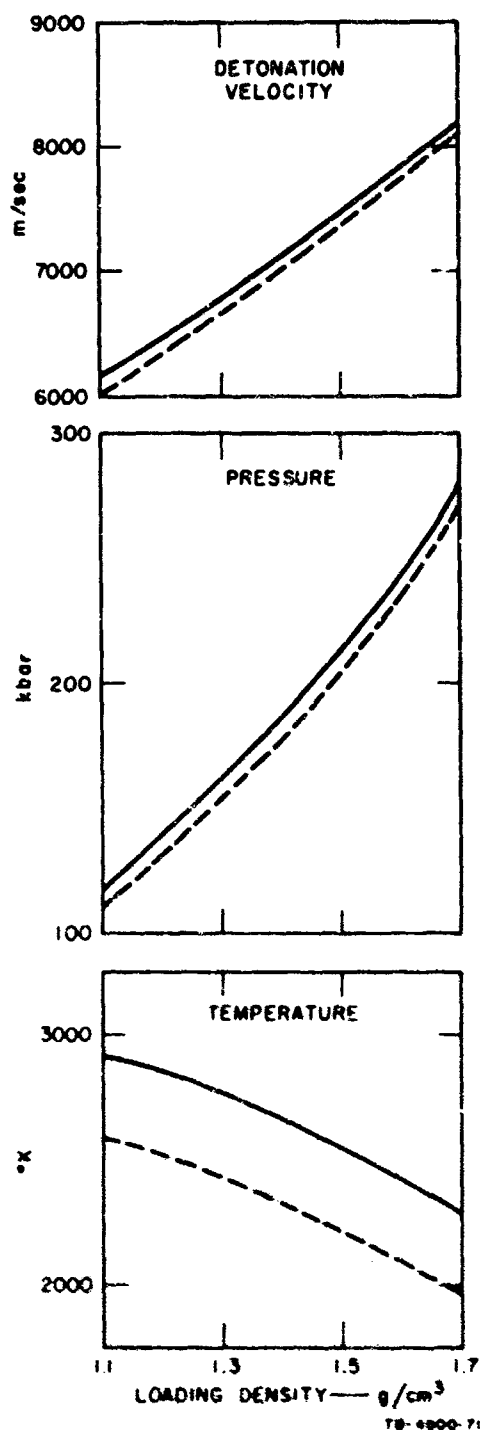
25

FIG. 2 CALCULATED DETONATION PARAMETERS FOR COMP B-3
AND 90/10 COMP B-3/OXAMIDE. The solid lines are for pure
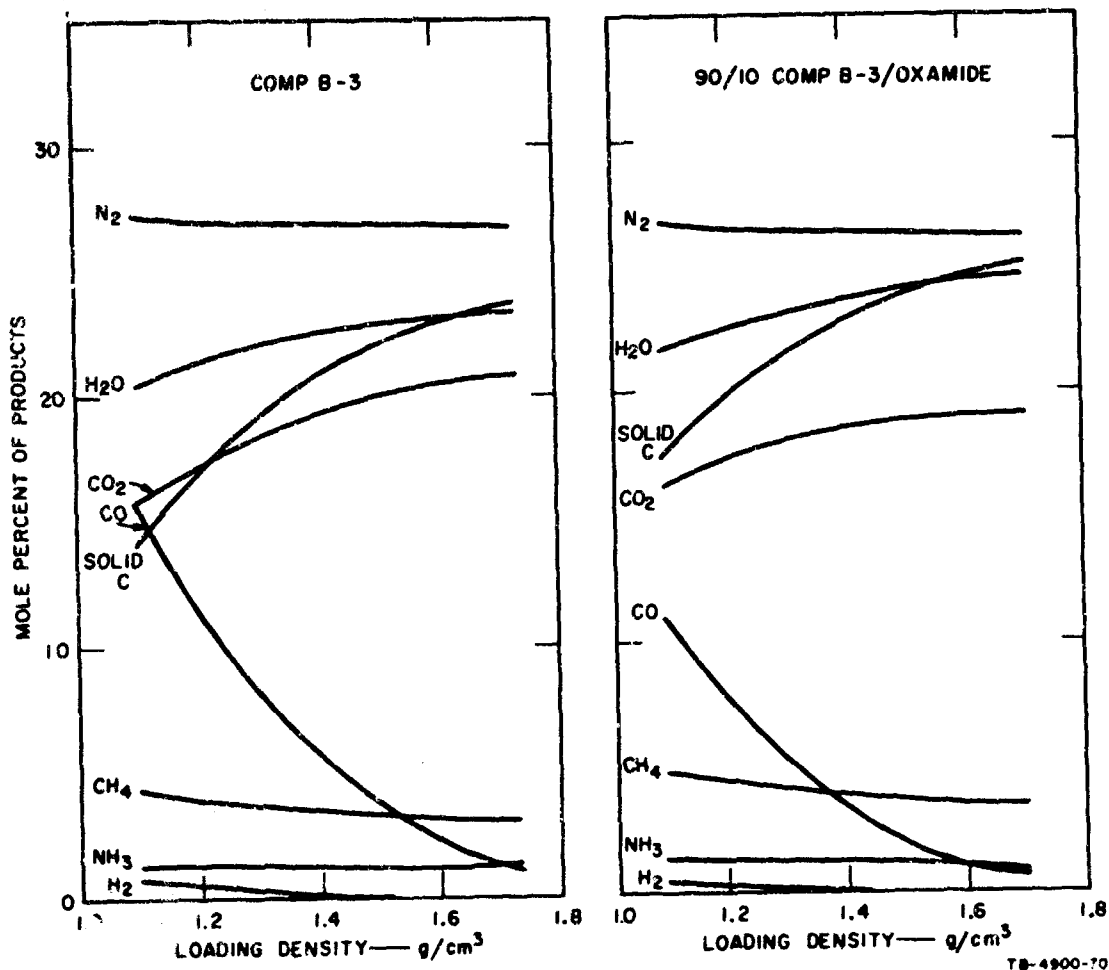Comp B-3 and the dashed lines are for Comp B-3 oxamide.

FIG. 3 DETONATION PRODUCTS OF COMP B-3 AND 90/10 COMP B-3/OXAMIDE

E. Calculations for TNT and Amatols

Flashing could be caused by the ignition of an agent-air mixture by burning detonation products. If the detonation products are incombustible, this cause of flashing is obviously eliminated. An explosive formulated to produce solely CO_2, H_2O, and N_2 is said to be oxygen-balanced and produces no combustible products.

Most military explosives have negative oxygen balance; i.e., they contain insufficient oxygen to convert all their carbon atoms to CO_2 and all their hydrogen atoms to steam. In industrial explosives ammonium

nitrate (AN) is commonly used as an energetic oxygen supplier. Ammonium
nitrate has several drawbacks such as hygroscopicity, a tendency to cake,
and a phase change at around $32^{\circ}C$ which produces a large volume increase.
Nevertheless, certain well-known mixtures containing AN could be valuable
in diagnostic tests of flashing mechanisms. It is for this reason that
we have made calculations for TNT, 50/50 TNT/AN, and 20/80 TNT/AN. The
TNT/AN mixtures are called amatols.

Since TNT is very deficient in oxygen, a large proportion of its
products will be combustible in air. The 50/50 amatol has slightly nega-
tive oxygen balance while the 80/20 amatol is very slightly oxygen-rich.
The results of the calculations (see Tables V and VI for input data) are
shown in Figs. 4 and 5. Rather surprisingly, T_1 for the amatols is cal-
culated to be substantially lower than that for the TNT. In part, this
is a consequence of the greater thermodynamic stability of the AN as com-
pared to TNT (more negative ΔH_f^o ; see Table VI), which results in a
smaller heat of reaction, Q_1, for the amatols than for TNT. Possibly
even more important is the fact that $\Sigma n_1 c_1$ increases substantially in
going from TNT to amatol. This also lowers T_1, since in the limit of a
perfect gas (Eq. 3) T_1 varies as $Q_1/\Sigma n_1 c_1$. The substantial increase in
calculated pressure of amatols over that of TNT (compared at a fixed ρ_0)
is puzzling. The interrelation of calculated parameters, e.g., the de-
pendence of P_1 on Q_1, will be examined in a later section.

F. Calculations of HMX and HMX/AN

For practical reasons as well as for the further diagnosis of flash-
ing, it may be desirable to have an explosive which produces a much higher
detonation pressure than the amatols but like the 20/80 amatol contains
no combustible products. As can be seen in Figs. 6 and 7 this objective
appears attainable with a 52/48 HMX/AN mix, which we call "Ametex." Again,
as for TNT and amatols, T_1 for HMX/AN is much lower and P_1 is slightly
higher than the corresponding values for HMX. This unexpected result will
be discussed later. The well-known explosive PBX 9404 consists of 94%
HMX and 6% binder.

Table VI

CALCULATION INPUT PARAMETERS FOR PURE EXPLOSIVES

Chemical Name	Formula	Formula Weight	Oxygen Balance(a)	Crystal Density (g/cc)	Heat of Formation ΔH_f^O (kcal/mole)	(kcal/g)
Pentaerythritol tetranitrate (PETN)	$C_5H_8N_4O_{12}$	316.2	-10.0	1.77	-125.0	-0.395
Cyclotrimethylene-trinitramine (RDX)	$C_3H_6N_6O_6$	222.1	-22.0	1.80	+ 14.71	+0.066
Cyclotetramethylene-tetranitramine (HMX)	$C_4H_8N_8O_8$	296.2	-22.0	1.90	+ 17.93	+0.061
Trinitrotoluene (TNT)	$C_7H_5N_3O_6$	227.1	-74.0	1.64	- 17.81	-0.078
Ammonium perchlorate (AP)	NH_4ClO_4	117.5	+34.1(b)	1.95	- 69.42	-0.591
Ammonium nitrate (AN)	NH_4NO_3	80.0	+20.0	1.73	- 87.27	-1.091

(a) Oxygen balance = $- \dfrac{1600}{\text{formula wt}} \left[2 \text{ C atoms} + \dfrac{H}{2} \text{ atom} - O \text{ atom.} \right]$
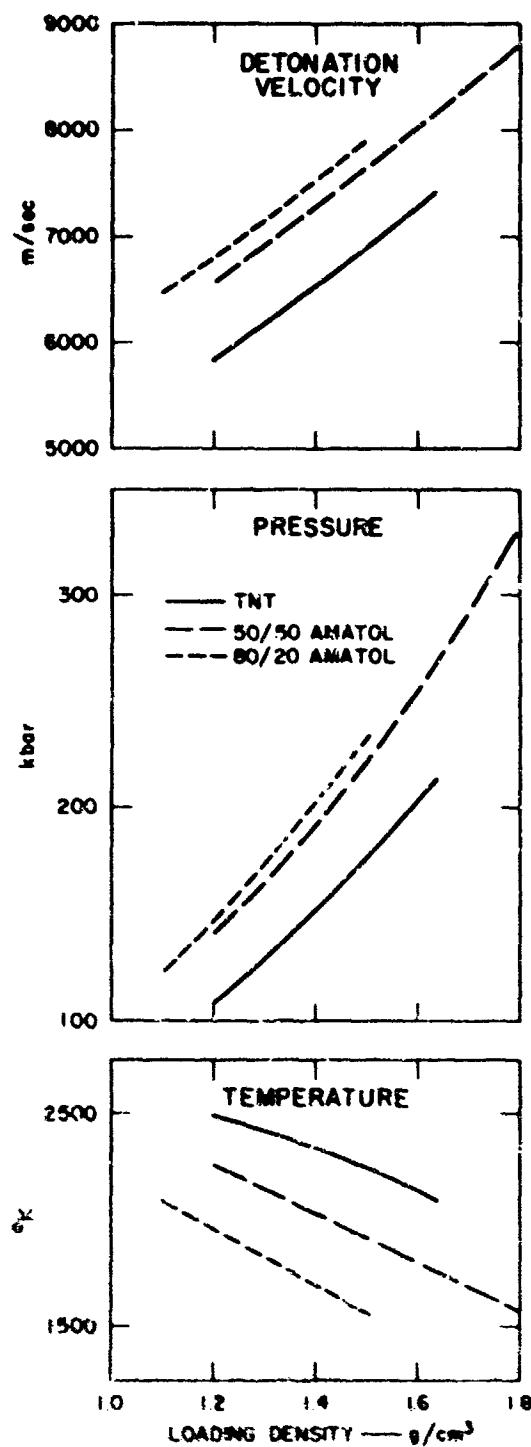
(b) Assuming Cl atoms form HCl.

FIG. 4 CALCULATED DETONATION PARAMETERS FOR
TNT, 50/50 AMATOL, AND 80/20 AMATOL. The
solid lines are for pure TNT, the dashed lines for 50/50
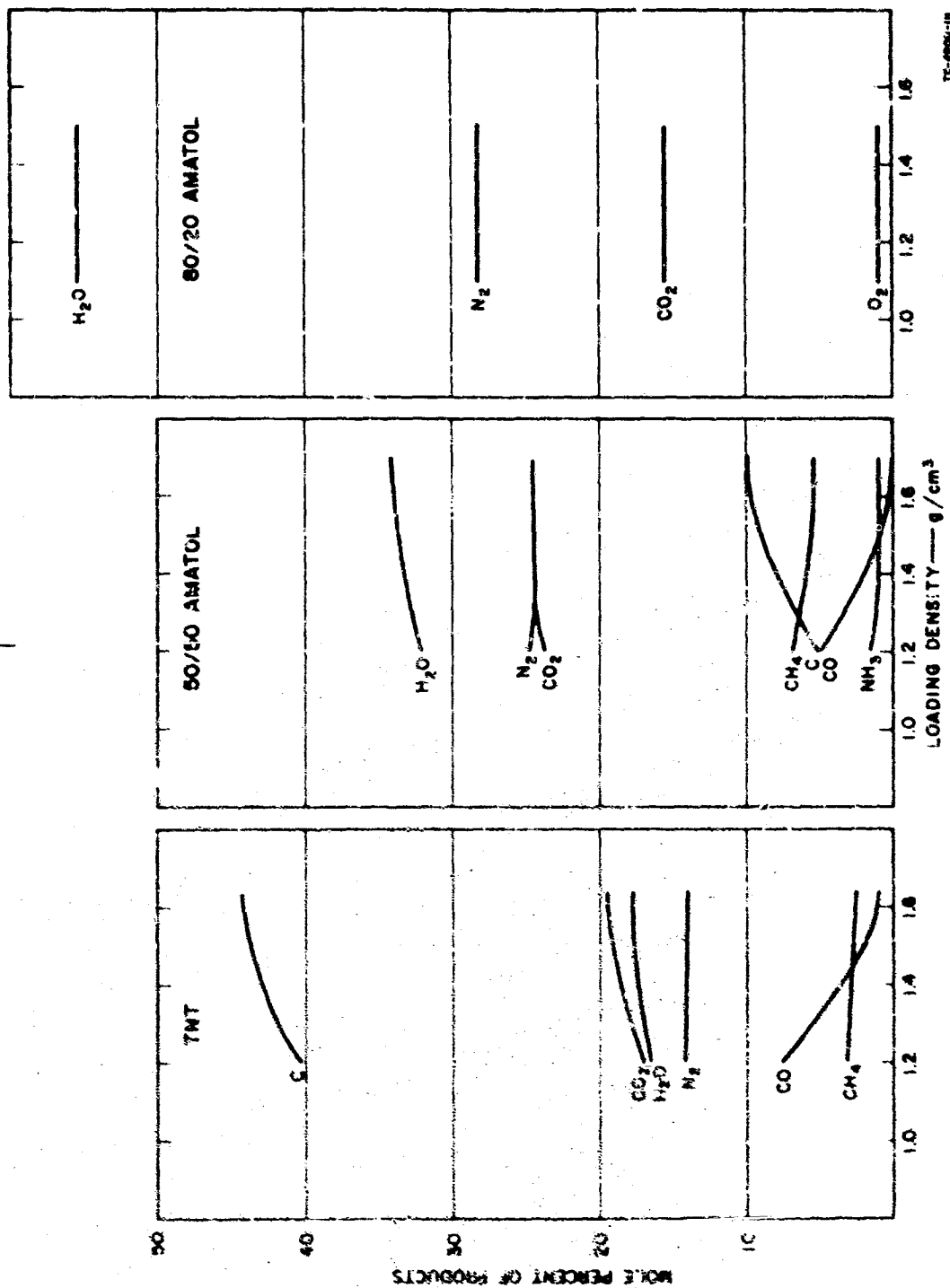amatol, and the dotted lines for 80/20 amatol.

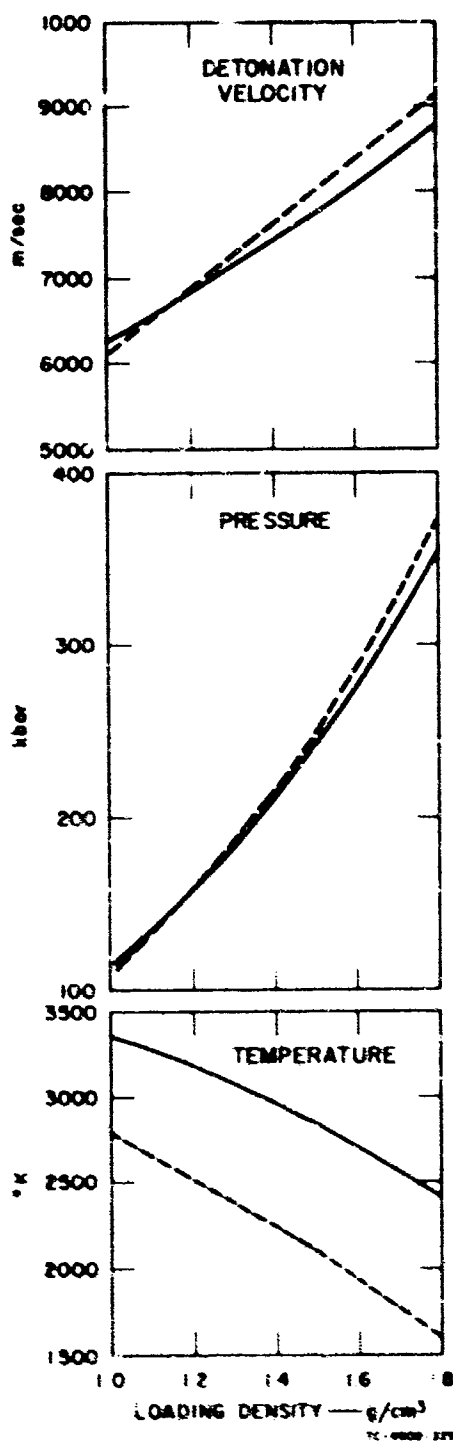FIG. 5 DETONATION PRODUCTS OF TNT, 50/50 AMATOL, AND 80/20 AMATOL

FIG. 6 CALCULATED DETONATION
PARAMETERS FOR HMX AND 52 48
HMX AN. The solid lines are for pure
HMX and the dashed lines are for 52 48
HMX/AN.

32

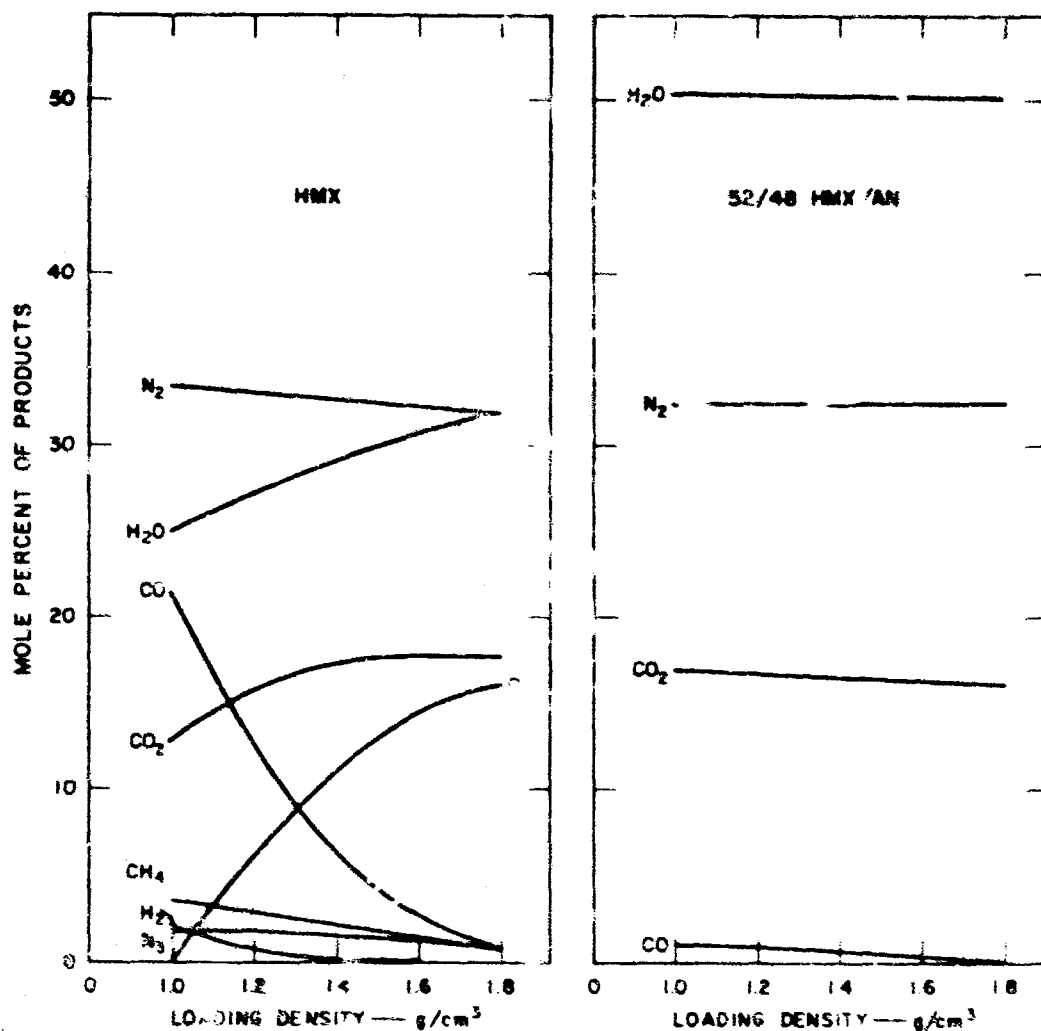FIG. 7 DETONATION PRODUCTS OF HMX AND 52/48 HMX/AN

G. Applicability of Detonation State Calculations to Flashing

At this point it will be instructive to reexamine the product composition versus ρ_e curves for oxygen-balanced explosives (Figs. 5 and 7). It is obvious that product composition for oxygen-balanced explosives is not influenced by the original loading density ρ_e, of the explosive.

33

Because ρ_0 strongly influences P_1, and to a lesser degree T_1, one must conclude that product composition for oxygen-balanced explosives is nearly independent of T_1 and P_1. This is a very important conclusion since it implies that product compositions calculated for the detonation state of oxygen-balanced explosives will remain essentially unchanged as these products expand.

Flashing probably occurs during or after detonation product expansion. Thus there is always the question of whether detonation state calculations are applicable to the flashing problem. This question is answered in the affirmative for oxygen-balanced explosives. For oxygen-poor explosives an unequivocal answer is not possible. RUBY product composition calculations along an expansion isentrope passing through the detonation equilibrium state are not very meaningful since the BKW equation must fail as the pressure decreases (see Section IIA). Nevertheless, such calculations have been made at LASL and at LRL, and they suggest, as might be expected from applying Le Chatelier's principle to the chemical equations b and c, that the main composition change during expansion (pressure decrease) is a decrease in solid carbon. For sufficiently great expansion there is of course a temperature drop as well as a pressure decrease. The temperature decrease implies that at some stage of the expansion the various chemical equilibria will "freeze" because the temperature of the system becomes too low to make further chemical readjustments sufficiently rapid.

Ornellas et al.[15] at LRL have estimated the temperature region below which equilibria are "frozen" to be 1500-1800°K, and they have measured the product composition of PETN detonated in a calorimeter and cooled to 25°C. In one set of experiments the PETN was confined so that in doing work on the confinement the temperature dropped rapidly. In an unconfined sample, because of reverberations at the calorimeter walls, the temperature dropped much more gradually than in the confined sample. Their results are compared with BKW calculations in Table VII.* It is apparent that the isentrope calculation (for "freeze-out" temperatures between 1500 and 1800°K) does not agree well with experiment. In fact it may be argued

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* We do not know of any other reliable product composition measurements other than the ones in Ref. 15.

34

Table VII

COMPARISON OF CALCULATED AND EXPERIMENTAL EXPANDED
PRODUCT COMPOSITIONS FOR PETN

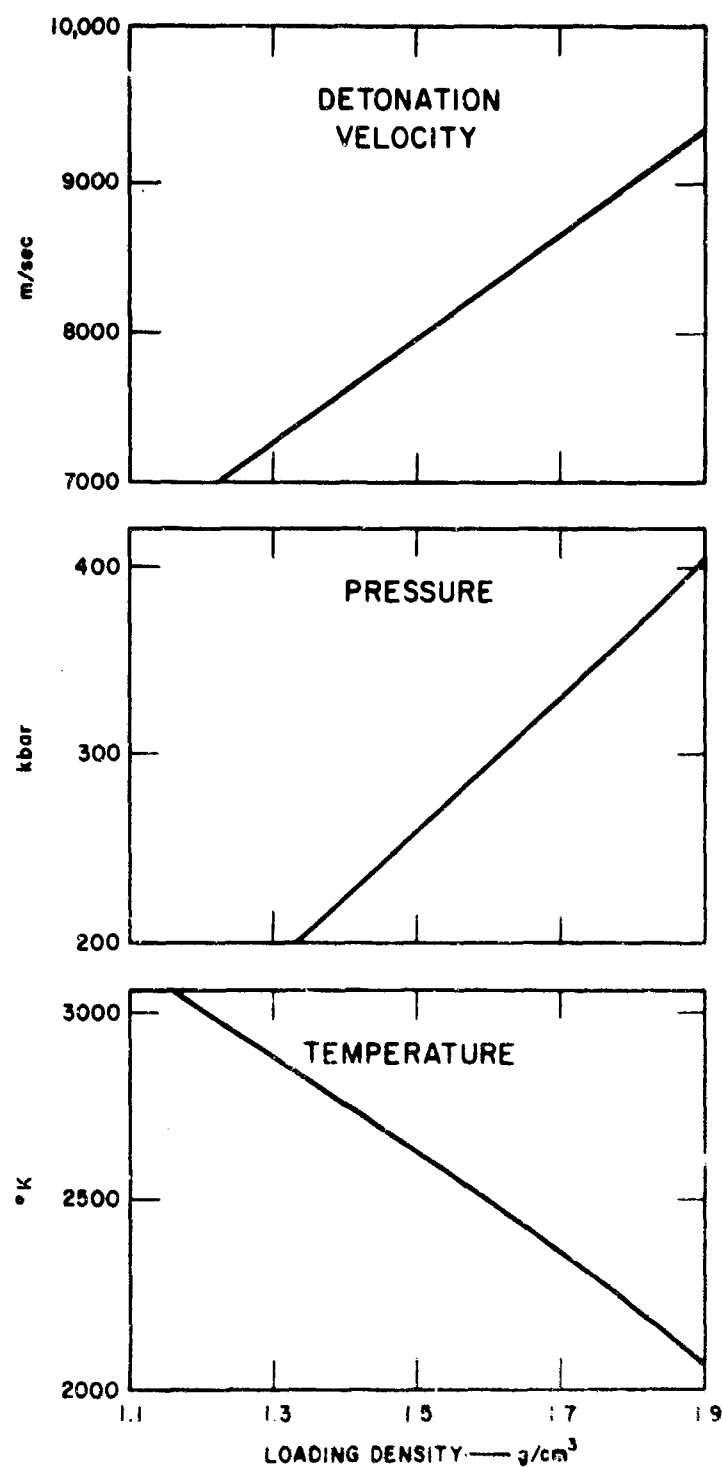|	Experimental		Calculated[2] for Detonation State		Calculated[15] for BKW Isentrope at 1500 to 1800°K
	Confined	Unconfined			
ρ_c (g/cc)	1.74	1.74	1.77	1.00	1.74
Products (mole/mole PETN)					
CO_2	3.38	3.50	3.95	3.04	4.0 to 4.1
CO	1.69	1.56	0.096	1.96	0.5 to 0.6
CH_4	0.003	<0.0002	<0.0002	0.0002	0.3 to 0.4
$C_{(s)}$	None	None	0.951	None	None
H_2O	3.50	3.45	4.00	3.94	3.2 to 3.3
H_2	0.45	0.51	<0.0002	0.050	0.02 to 0.05
NH_3	0.037	<0.0002	<0.0002	0.004	0.04 to 0.06
N_2	2.00	2.00	2.00	1.99 +	2.0

that a detonation state calculation for low packing density PETN, also
shown in Table VII, agrees with experiment about as well as the isentrope
calculation. All this still leaves unanswered the question of the ap-
plicability of detonation state calculations (for oxygen-negative ex-
plosives) to the expanded state. It suggests that a crude estimate of
expanded product composition may be made from detonation state calcula-
tions for explosives at low packing density.

H. Calculations for HMX and HMX/AP

In Section IIF it was shown that an energetic explosive containing
no combustible products can be made by mixing HMX and AN. This mixture,
however, would be unsuitable for military use because of the poor storage
qualities of AN. It is believed that a practical military explosive can
be made from mixtures of HMX and ammonium perchlorate (AP) imbedded in
a suitable plastic matrix. Calculations for the oxygen-balanced 61.2/38.8
HMX/AP mixtures are shown in Figs. 8 and 9. Comparing these results with
the calculations for HMX, given in Figs. 6 and 7, shows that P_1 is greater
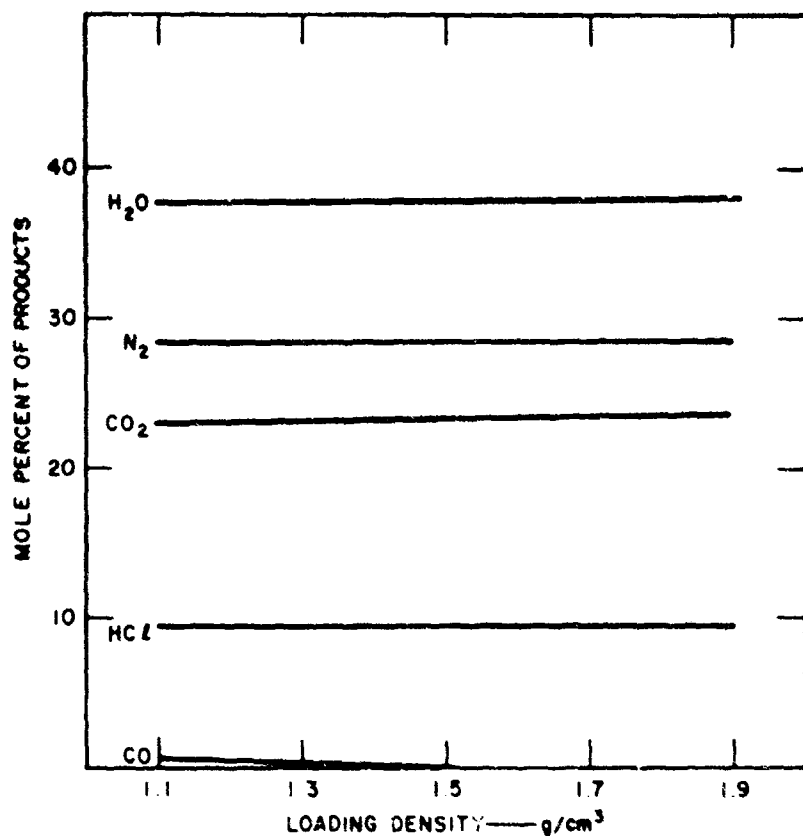and T_1 is less for HMX/AP.

I. Flashing Mechanism

Several investigations[14,16,17] suggest that flashing results pri-
marily from the ignition of an agent-air mixture by burning of detona-
tion products. Combustible mixtures in air for either products or agent
are formed only after the whole system has undergone a considerable degree
of expansion. The energy transport from the hot burning products to the
still unignited agent-air mix is presumably via conduction, convection,
and radiation, all of which are slow compared to hydrodynamic transport
phenomena. The detonation temperature T_1 is rapidly quenched if detona-
tion products expand and do work on their surroundings. Thus ignition
of agent-air mixtures by heat transport is most unlikely if the only
source of high temperature is T_1. However, afterburning of detonation
products in air can maintain regions of high temperature (of the order
of T_1 or even higher) for times sufficiently long to allow appreciable
heat transport to the agent-air mix. Detonation products that are in-
combustible can no longer act as an energy stimulus of sufficiently long
duration to ignite the agent-air mixture.

FIG. 8 CALCULATED DETONATION PARAMETERS FOR
61.2/38.8 HMX/AP

FIG. 9 DETONATION PRODUCTS OF 61.2/38.8 HMX/AP

There appears to be insufficient time for enough heat transfer, from essentially unexpanded detonation products to the agent, to cause flashing. In any event most agents per se, and not as agent-air mixtures, would be difficult to ignite. However, if T_1 is very large, it is conceivable that enough heat can be transferred to the agent to cause some of it to degrade (e.g., pyrolize), without emitting light, before T_1 is drastically reduced by expansion.

There is yet another possible agent degradation mechanism in which the shock sent into the agent by the detonating explosive creates hot regions of sufficiently high temperature to cause degradation.

It may be desirable to assess the relative importance of these degradation schemes. To that end we have listed in Table VIII various explosive compositions that could be used for diagnostic tests. The choice of the explosives was made on the basis of our calculations as well as published calculations of others. All explosive parameters are rated relative to Comp B, the presently used dissemination charge.

J. Interrelation Among Calculated Detonation Parameters

It is most desirable to be able to check the internal consistency of the results of an involved computational procedure such as RUBY. Such checks should be capable of pointing out errors in input data and/or machine malfunctioning. The most obvious and least ambiguous check is naturally that of mass balance; i.e., all atoms originally present must appear in the calculated products. A correct mass balance is a necessary but not a sufficient condition for the internal consistency of the calculation. Other checks are needed in the usual case where there are no experimental data to compare with the calculation.

As shown in the appendix, a simple relation between Q_1 and P_1 is obtained if the EPv equation of state is $E = Pv/\Gamma - 1$, where Γ is $-(\partial \ln P/\partial \ln v)_S$. This relation is:

$$P_1 \sim 2\rho_0 Q_1(\Gamma - 1) \tag{10}$$

Many calculations[8,12] give $\Gamma \sim$ constant ~ 3. Thus, according to Eq. (10), a plot of P_1 versus $\rho_0 Q_1$ should be a straight line of slope $2(\Gamma - 1)$. Experimental and calculated P_1's are plotted versus computed $\rho_0 Q_1$'s in Fig. 10. Actually the slightly more accurate $\rho_0 [Q_1 + n_1 R T_0 (\Gamma/\Gamma - 1)]$ was used rather than $\rho_0 Q_1$. Most of the points lie along a line of the expected slope, $2(\Gamma - 1)$, with $\Gamma \simeq 3$, but the line does not pass through the origin. This implies that Eq. (10) should contain an additional constant and that the simple EPv equation of state used in the appendix is not consistent with the BKW equation of state.

In Section IIA it was shown that, if P_1 is large, product composition and consequently Q_1 can be estimated fairly accurately strictly

Table VIII

COMPARISON OF POSSIBLE DISSEMINATION TEST EXPLOSIVES
WITH COMP B ($\rho_0 = 1.6$ g/cm^3)

HE	Function	Pressure	Temperature	Combustibles
90/10 Comp B/oxamid (1.6 g/cc)	To reduce temperature	~ same	lower	same
Nitroguanidine (1.6 to 1.7 g/cc)	To reduce temperature	~ same	much lower	lower
Hydrazine nitrate (~1.6 g/cc)	To reduce temperature	slightly lower	much lower	none(a)
TNETB (~1.6 g/cc)	To reduce combustibles	~ same	higher	lower
80/20 TNETB/B:NEN (~1.7 g/cc)	To reduce combustibles	~ same	higher(b)	none
52-48 HMX/AN (1.8 g/cc)	To reduce combustibles	higher	probably lower	none
HMX (1.8 g/cc)	To increase pressure	higher	somewhat lower	lower
52/48 HMX/AN (1.8 g/cc)	To increase pressure	higher	probably lower	none
Nitroguanidine (~1.4 g/cc)	To reduce pressure	lower	probably lower	lower
80/20 Comp B/Al (1.8 g/cc)	To increase temperature	lower	much higher	many more

(a) There is even some oxygen in the products.
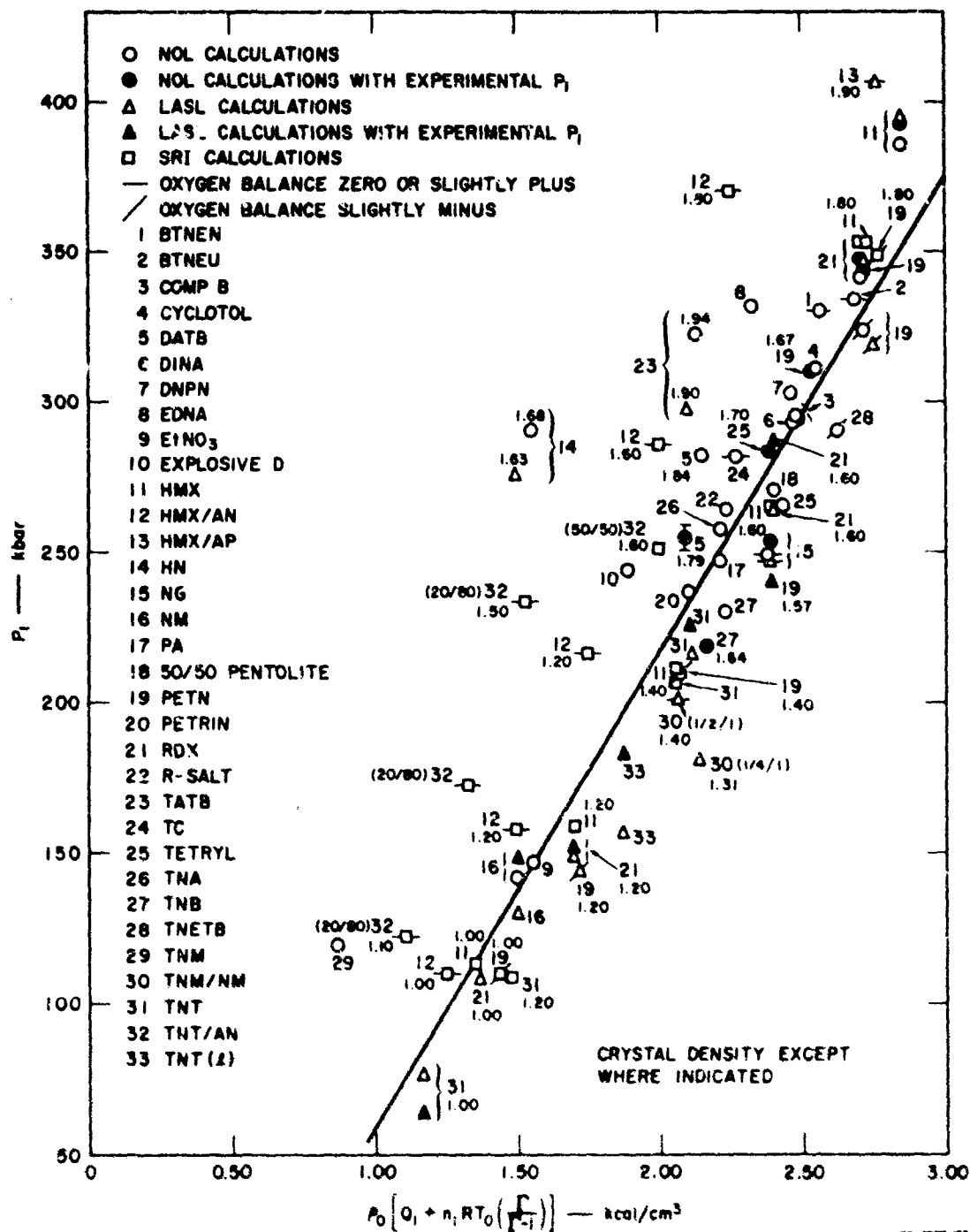(b) About the same as for TNETB.

40

FIG. 10 CORREIATION BETWEEN DETONATION PRESSURE AND HEAT OF REACTION

on the basis of mass balance and thermochemistry, i.e., without recourse
to any PvT equation of state. Thus the plot of Fig. 10, regardless of
its theoretical significance or lack of it, provides a method of corre-
lating most of the computed and experimental $P_1 - Q_1$ results. For the
LASL-NOL computations,[9],[12] only TNM and HN do not fit the proposed corre-
lation. Both of these materials are oxygen-rich and have small Q_1's.
Other oxygen-rich materials such as BTNEN, NG, and TC (see Fig. 10) fall
close to the proposed correlation. In our calculations all oxygen-balanced
or slightly oxygen-rich materials have a higher P_1 than the proposed corre-
lation would predict for their respective Q_1's. Since we expect all Q_1's
to be reasonably correct, this could indicate that our RUBY computations
for oxygen-balanced mixtures somehow give P_1's that are too high—a con-
clusion that is not entirely unexpected. The necessary "curve-fitting"
for RUBY and BKW codes was done using the oxygen-poor RDX and TNT as
"standard" explosives. The equation of state parameters (ψ, β, etc.)
from this fit may not be applicable to oxygen-balanced mixtures. Moreover,
the co-volumes (α_i of Eq. 9) for H_2O and CO_2 used in our calculations are
larger than those used by LASL and NOL (see Table II). Consequently, the
differences between SRI and LASL-NOL calculations for oxygen-balanced
explosives, whose products contain large proportions of H_2O and CO_2, may
reflect this co-volume difference.

III CONCLUSIONS AND RECOMMENDATIONS

If flashing is caused by ignition of agent-air mixtures by after-burning detonation products of the dissemination charge, then flashing can be eliminated by:

1. Formulating the explosive charge to produce incombustible products.

2. Designing the munition so that detonation products expand symmetrically. During expansion the products do work on the surroundings and are cooled before they come into contact with the air. It has been shown[14] that Comp B charges do not flash if they are symmetrically surrounded by agent simulant and symmetrically detonated.

3. Using explosives of low detonation temperature to help reduce flashing. This approach appears to be much less promising than 1 or 2. In any event it appears desirable to keep detonation temperatures low. Even if no flashing is observed a high detonation temperature could cause localized degradation of the agent.

The easiest and surest way to formulate explosives producing incombustible products is to include sufficient oxygen-containing compounds in the original explosive to convert all the carbon atoms and hydrogen atoms of the explosive to CO_2 and H_2O. Excess oxygen should be avoided as it may interact with the agent. Ideally the oxygen-balanced explosive should be a single compound, e.g., ethylene glycol dinitrate, since this avoids all problems of product nonuniformity due to: (1) nonuniform and/or insufficiently intimate mixing of explosive constituents and (2) different chemical reaction rates for the various compounds in the mixture. Unfortunately, for military uses the requirement of an oxygen-balanced single compound is too restrictive. It seems better to consider oxygen-balanced mixtures but to exercise great care in selecting and preparing them.

The preceding sections have demonstrated that the products of an oxygen-balanced explosive, provided equilibrium is achieved, are not affected by initial density, expansion of the products, or even the method of calculation. The other computed detonation parameters, such as pressure or temperature, of course depend on the method of calculation. At present, any computed detonation temperatures must be accepted with considerable skepticism. However, viewed in terms of the fundamental physics involved, temperature calculations based on the BKW equation of state are inherently more plausible than calculations based on modified Abel equations of state. The present RUBY code is too inflexible to permit the use of other equations of state than BKW, which, as has been discussed, has serious theoretical shortcomings. A very general computational code, now being completed at SRI, will be much more flexible than RUBY. This new code should be employed to develop a theoretically sound equation of state, to test it against available data, and to suggest areas (possibly temperature measurements) where new data must be obtained.

Shock heating of the agent by the detonating dissemination charge may cause localized agent degradation. RUBY usually provides reliable estimates of detonation pressure. Thus from RUBY results one can suggest explosives for diagnostic tests of the importance of shock heating (Table VII).

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GLOSSARY

b	Second virial coefficient
C	Local sound velocity
c	Specific heat at constant volume
D	Detonation velocity
E	Internal energy
ΔH_f^o	Standard heat of formation
K	Thermodynamic equilibrium constant
n	Number of moles per gram of explosive
P	Total pressure
p	Partial pressure
Q	Heat of reaction per gram of explosive
R	Universal gas constant
T	Temperature, $^o K$
u	Particle velocity
v	Specific volume
α	Co-volume
γ	Ratio of specific heat constant pressure and constant volume
ρ	Density
ψ	Scaling factor

Subscripts

0	Original, unreacted explosive
1	Equilibrium detonation state
S	Constant entropy

APPENDIX

From the conservation equations for a one-dimensional shock,

$$E_j - E_0 = \frac{1}{2} P_j (v_0 - v_j) \qquad \text{(A-1)}$$

if $P_j \gg P_0$. The subscript j refers to the equilibrium detonation state (the Chapman-Jouguet state), the subscript 0 refers to the unreacted explosive at initial temperature and pressure, and the subscript 1 refers to equilibrium detonation products which are not necessarily at P_j and T_j. For explosive $(T_0, F_0) \rightarrow$ equilibrium detonation products (T_0, P_0),

$$\Delta E = Q_1 + n_1 R T_0 = E_0(T_0, P_0) - E_1(T_0, P_0) \qquad \text{(A-2)}$$

Since $E_j = E_1(T_j, P_j)$ and $E_1 = E_0(T_0, P_0)$, Eq. (A-2) gives

$$E_j - E_0 = E_1(T_j, P_j) - E_1(T_0, P_0) - \Delta E$$

and substituting in Eq. (A-1) results in

$$\frac{1}{2} P_j (v_0 - v_j) = E_1(T_j, P_j) - E_1(T_0, P_0) - \Delta E \qquad \text{(A-3)}$$

The Chapman-Jouguet condition is expressed by

$$v_j/v_0 = \rho_0/\rho_j = \Gamma/(\Gamma + 1) \qquad \text{(A-4)}$$

where

$$\Gamma \equiv - \left(\frac{\partial \ln P}{\partial \ln v} \right)_S$$

For the so-called polytropic gas, at constant entropy S, $P = A\rho^{\Gamma}$ where $A = A(S)$. Under certain conditions[12],[18] this leads to the following EPv equation of state

$$E = \frac{Pv}{\Gamma - 1} \tag{A-5}$$

Combining Eqs. (A-3), (A-4), and (A-5) results in

$$\frac{P_j v_0}{(\Gamma + 1)}\left[\frac{\Gamma}{\Gamma - 1} - \frac{1}{2}\right] = \frac{P_j v_0}{2(\Gamma - 1)} = \Delta E + \frac{P_0 (v_0)}{\Gamma - 1} \tag{A-6}$$

If the detonation products at (P_0, T_0) are perfect gases, Eq. (A-6) is further simplified to

$$\frac{P_j v_0}{2(\Gamma - 1)} = \Delta E + \frac{n_1 RT}{\gamma - 1} = Q_1 + n_1 RT_0 \left(1 + \frac{1}{\gamma - 1}\right) = Q_1 + \frac{n_1 RT_0 \gamma}{\gamma - 1}$$

or

$$P_j = 2\rho_0 (\Gamma - 1)\left[Q_1 + n_1 RT_0 \frac{\gamma}{\gamma - 1}\right] \sim 2\rho (\Gamma - 1)Q_1 \tag{A-7}$$

since $Q_1 \gg n_1 RT_0 \gamma/\gamma - 1$ in most cases. Thus for a consistent set of dimensions (cgs) a plot of P_j versus $\rho_0 Q_1$ should be a straight line of slope $2(\Gamma - 1)$, since $\Gamma \sim$ constant ~ 3.